Temporal Evolution of Nano-ordered structures in Nickel-based Superalloys by Kinetic Monte Carlo Simulations

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- The **nucleation, growth and coarsening** of new ordered phases is studied by kinetic Monte Carlo simulations.
- The **thermodynamic parameters** are confirmed by the **consistency** of a ternary isothermal phase diagram calculated with Grand Canonical Monte Carlo simulations with an experimental one (Taylor, 1952).
- Two **filter** parameters are used to differentiate phase separation and ordered phas formation: **iso-order** (Warren-Cowley) and **isoconcentration**
- The **nucleus** of the first precipitates that form exhibit **short-range order.** The first precipitates are **Cr-rich** and the composition is close to Ni_3Cr.
- Initially two different structures of ordered $Ni_3Cr_{1-x}Al_x$ precipitates exist -- DO_{22} and $L1_2$.
- **Al-rich** $Ni_3Al_{1-x}Cr_x$ ordered are evolving from **Cr-rich** $Ni_3Cr_{1-x}Al_x$ $L1_2$ ordered phase.
- The **kinetic pathway** of the compositions of precipitates is determined. **Three different populations** are observed.